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RCM STUDIES TO ENABLE GASOLINE-RELEVANT LOW TEMPERATURE COMBUSTION

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Project ID # ACS054
FY2018 DOE Vehicle Technologies Program Annual Merit Review
Advanced Combustion Engine R&D
Wednesday, June 19, 2018
Program Managers: Gurpreet Singh, Michael Weismiller

OVERVIEW

Timeline

- Project started FY 2011
- Project directions and continuation reviewed annually, and in FY 2019 VTO Lab Call

Barriers

- Lack of fundamental knowledge of advanced combustion engine regimes
- Lack of modeling capability for combustion and emission control

Budget

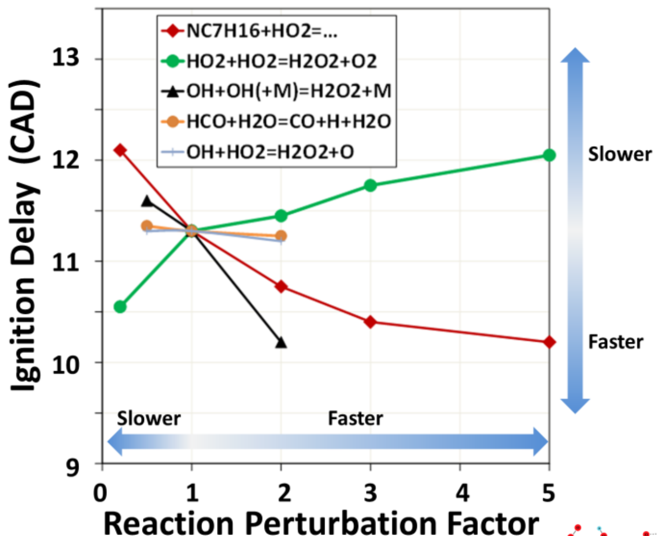
- Project funded by DOE / VTP
  → FY 2016 funding: $490 k
  → FY 2017 funding: $370 k
  → FY 2018 funding: $370 k

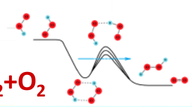
Partners

- ANL – Lead, Goldsborough (PI)
- LLNL – gasoline surrogate model, simulation tools
- TCD – surrogate methodologies
- SNL – RD5-87 gasoline, HCCI engine data
- International RCM Workshop

OBJECTIVES AND RELEVANCE TO DOE

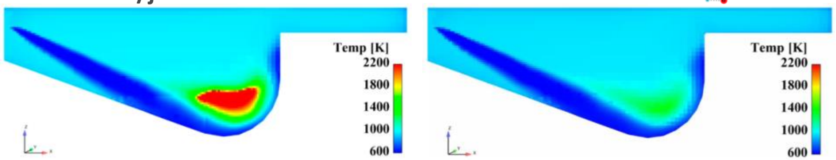
- Acquire fundamental data, and help develop / validate / refine chemical kinetic and relevant models for transportation-relevant fuels (conventional and future gasolines, diesels and additives) at conditions representative of advanced combustion regimes, leveraging collaborations with researchers across the broader community.
- Predictive simulations with such models, which require low associated uncertainties, could be utilized to overcome technical barriers to low temperature combustion (LTC), and achieve required gains in engine efficiency and pollutant reductions.





doi:10.1021/jz400874s

$HO_2+HO_2=H_2O_2+O_2$



PROJECT MILESTONES

FY 2018

Task	Milestone	Status
1	Acquire new ignition measurements for multi-component surrogate blends to mimic ‘neat’, and ethanol-blended gasolines (E0–E30); Evaluate, quantify performance of surrogate formulation approaches.	ongoing
2	Acquire ignition measurements for full boiling-range gasoline, RD5-87 (an E10 gasoline).	✔
3	Acquire ignition measurements for CRC AVFL31b project (four full boiling-range gasolines).	ongoing
4	Acquire ignition measurements of single-component aromatics, and olefins; probe synergistic/antagonistic behavior of binary blends.	FY18–Q4
5	Coordinate RCM Workshop 2nd Characterization Initiative, CFD activities, and organize 4th International RCM Workshop (Dublin, IRELAND)	FY18–Q4
6	~~Extend UQ/GSA framework and investigation to consider additional targets beyond ignition delay times, including heat release rates~~	postponed

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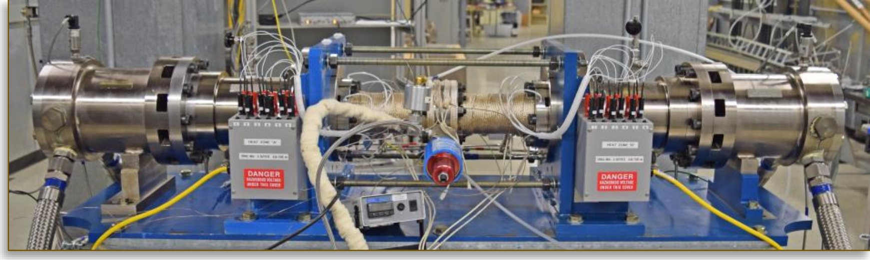
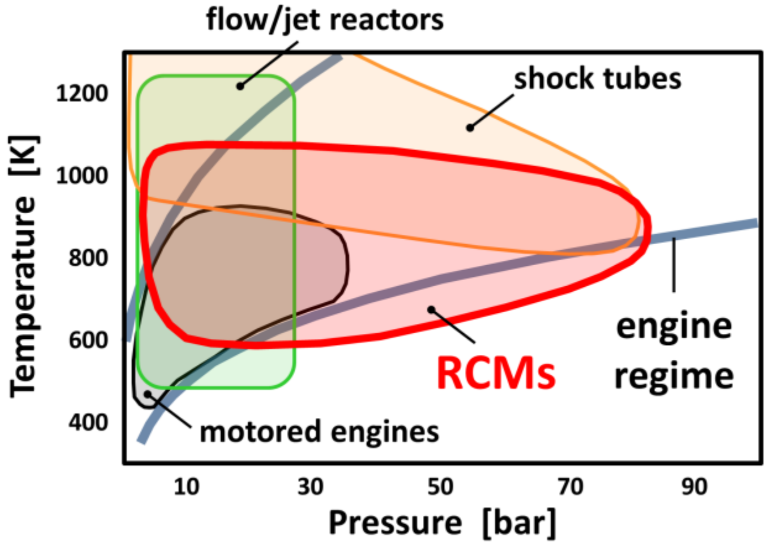
PROJECT APPROACH

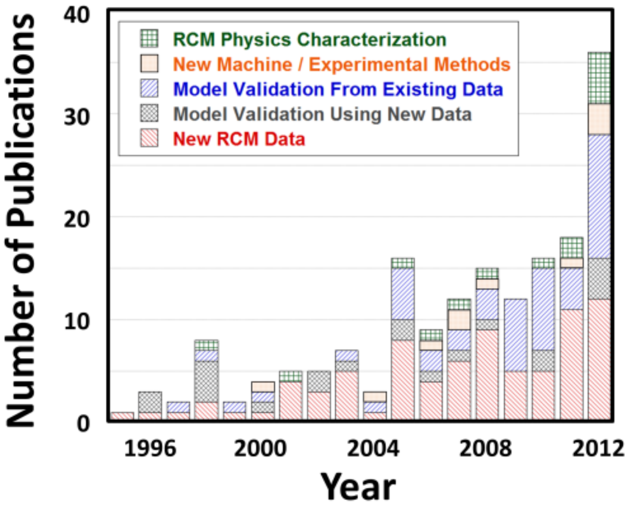


PROJECT APPROACH

Rapid Compression Machine

- Utilize ANL's twin-piston RCM to acquire autoignition data





- Employ novel data analysis tools and advanced diagnostics
  – Physics-based, reduced-order system model;
  – Developing capabilities to better probe chemistry.
- Synergistically improve kinetic models using analysis techniques (e.g., UQ/GSA) and detailed calculations/measurements of sensitive processes (e.g., individual reaction rates)

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TECHNICAL ACCOMPLISHMENTS / PROGRESS

TECHNICAL ACCOMPLISHMENTS / PROGRESS

Twin-Piston Rapid Compression Machine

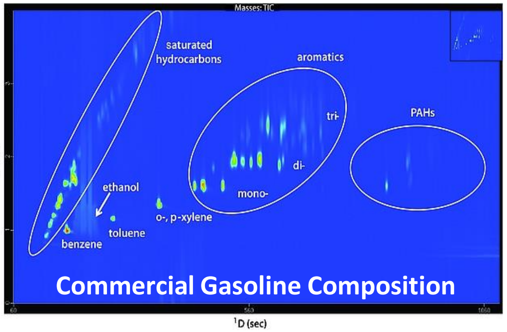
- Modifications and upgrades implemented since FY 2017 AMR to improve measurement capabilities
  - LVDT mounts for dynamic tracking of pistons fabricated, preliminary testing completed; full implementation postponed to FY18-Q4;
  - New seals for increased wear resistance acquired and tested; thermal cycling of machine led to unexpected wear / excessive leakage;
  - Calibration protocol devised for Kistler combustion transducer; daily monitoring compared against historical records to track performance, identify problems.
- Operational challenges exist
  - Synchronous twin-piston operation difficult to achieve; typically ~2-3 ms difference in actuation. Some variability over multiple days of testing. Affects primarily short (τ < 2 ms) ignition delay times; can introduce noise / perturbations into heat release analysis, complicating quantification of LTHR/ITHR.

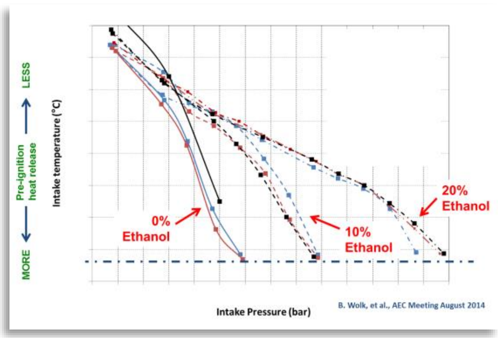
TECHNICAL ACCOMPLISHMENTS / PROGRESS

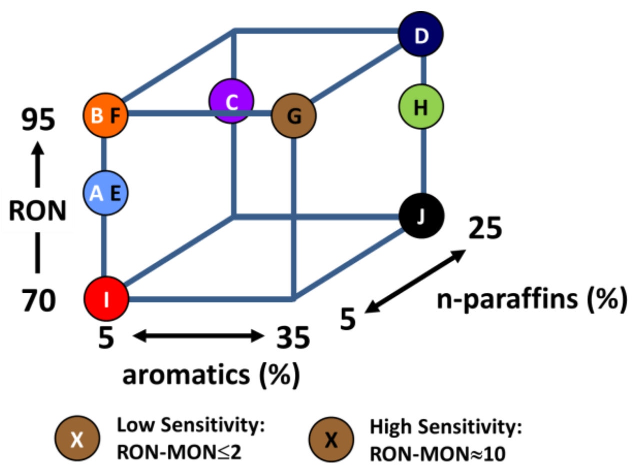
Investigating Gasoline and Surrogates

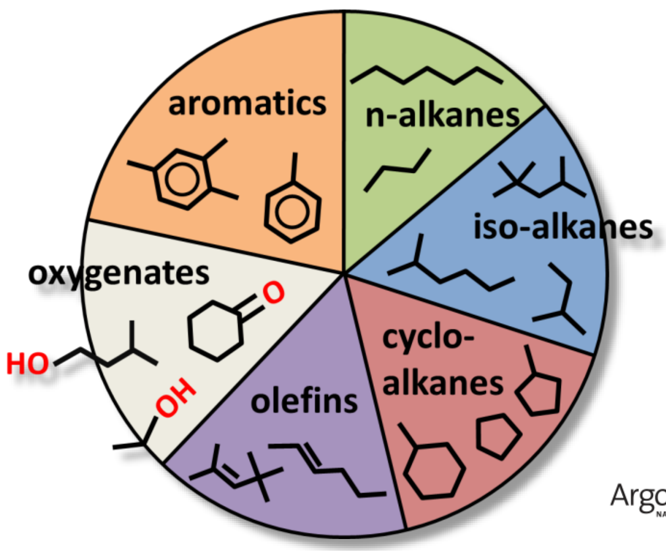
- Predictive modeling of LTC needed to guide design
  - Gasoline is complex, compositionally variant
    - → How do these features affect LTC behavior, especially autoignition phenomena at low and intermediate temperatures (T = 600–1100 K)?
    - → How can real fuels be represented by multiple-component (3-10) formulations?
    - → Data are needed to compare autoignition behavior of real, full boiling range fuels with surrogates, including individual components, blends of these and mixtures with ethanol.

http://www.sigmaaldrich.com/catalog/product/supelco/g006346



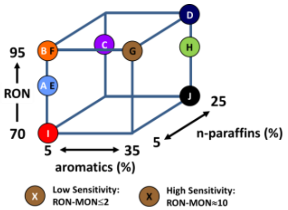


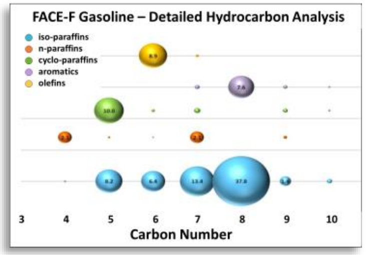




TECHNICAL ACCOMPLISHMENTS / PROGRESS

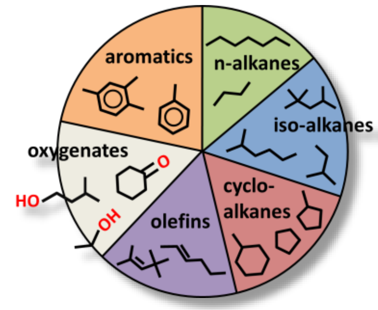
Task 1 – Gasoline / Ethanol Blends





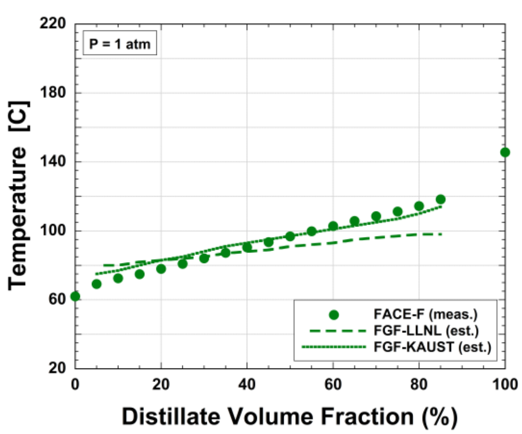
- FACE-F used as representative gasoline
  - Composition, properties well-characterized;
  - Investigating various approaches to formulate multi-component surrogate mixtures, measuring influence of ethanol (blending levels of E0–E30) on autoignition chemistry; quantifying τ, LTHR/ITHR changes.

Property	FACE-F	PRF 91.5	TPRF-F	FGF-LLNL	FGF-KAUST
RON	94.4	91.5	94.4	93.8	93.6
MON	88.8	91.5	89.1	89.5	88.9
S	5.6	0	5.3	4.3	4.7
Density (g/mL)	707	694	755	712	707
H/C	2.13	2.25	1.84	2.06	2.12
Avg. MW (g/g-mol)	94.8	112.9	103.9	100.2	96.2
Branching Index	0.68	0.55	0.69	0.51	0.50



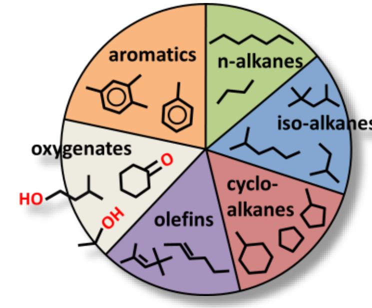
Component	PRF 91.5	TPRF-F	FGF-LLNL	FGF-KAUST
n-Butane	0	0	0	6.9
2-Methyl butane	0	0	0	9.8
2-Methyl hexane	0	0	0	7
Cyclopentane	0	0	14	15.8
1,2,4-Trimethyl benzene	0	0	0	8.4
1-Hexene	0	0	14	8.4
n-Heptane	9.5	11.1	7	0
2,2,4-Trimethyl pentane	90.5	49.1	53	43.7
Toluene	0	39.8	12	0

Mole percentages of components in surrogate blend

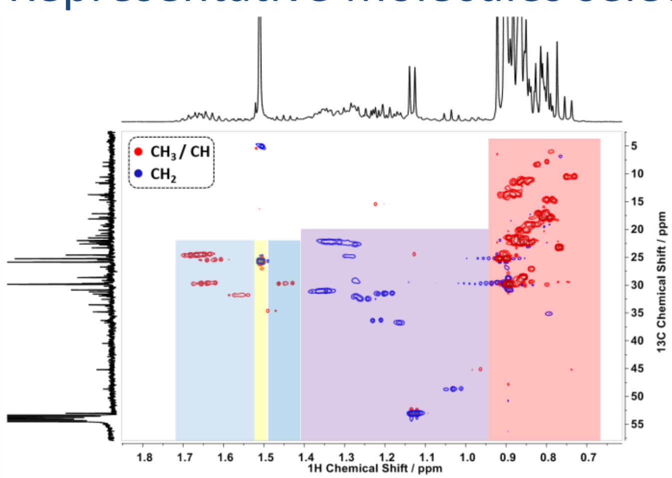


TECHNICAL ACCOMPLISHMENTS / PROGRESS

Task 1 – Gasoline / Ethanol Blends



- State-of-the-art methodologies employ:
  - Hydrocarbon-class based approach with representative molecules to match paraffinic, olefinic, etc. content
  - Compositional refinement to match H:C (MW), liquid density, RON/MON and distillation curve (typically predicted via correlations)
- FY2017 data highlighted inadequacies for capturing blending effects
- Functional-group methodology targeted for improved performance
  - ^{1}H and ^{13}C NMR used to quantitatively determine functional group composition of full boiling-range fuels (Trinity College Dublin)
  - Representative molecules selected to match group distributions

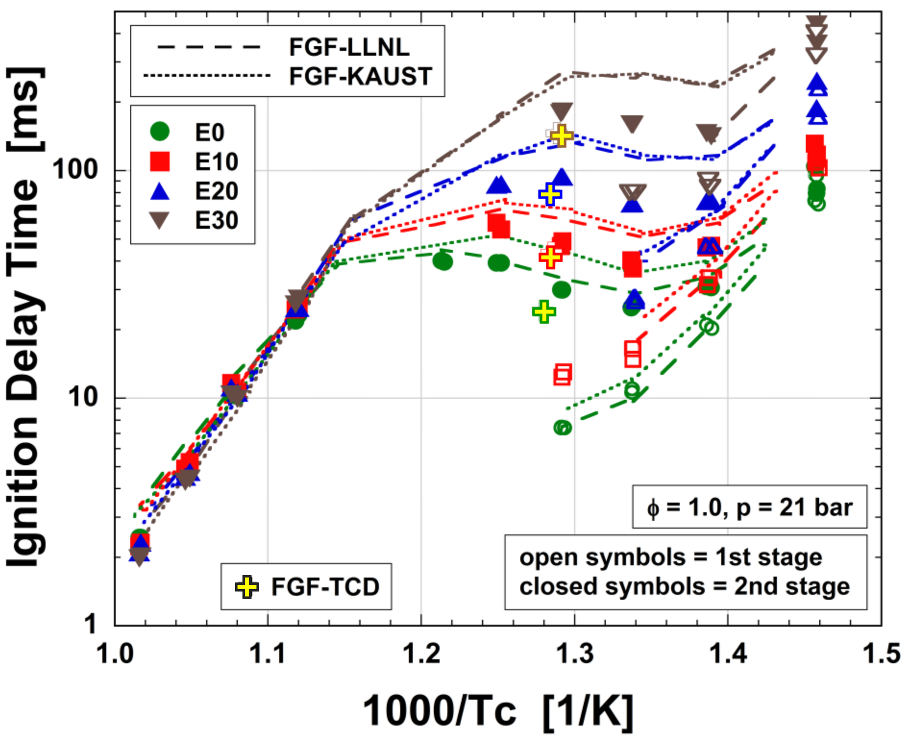


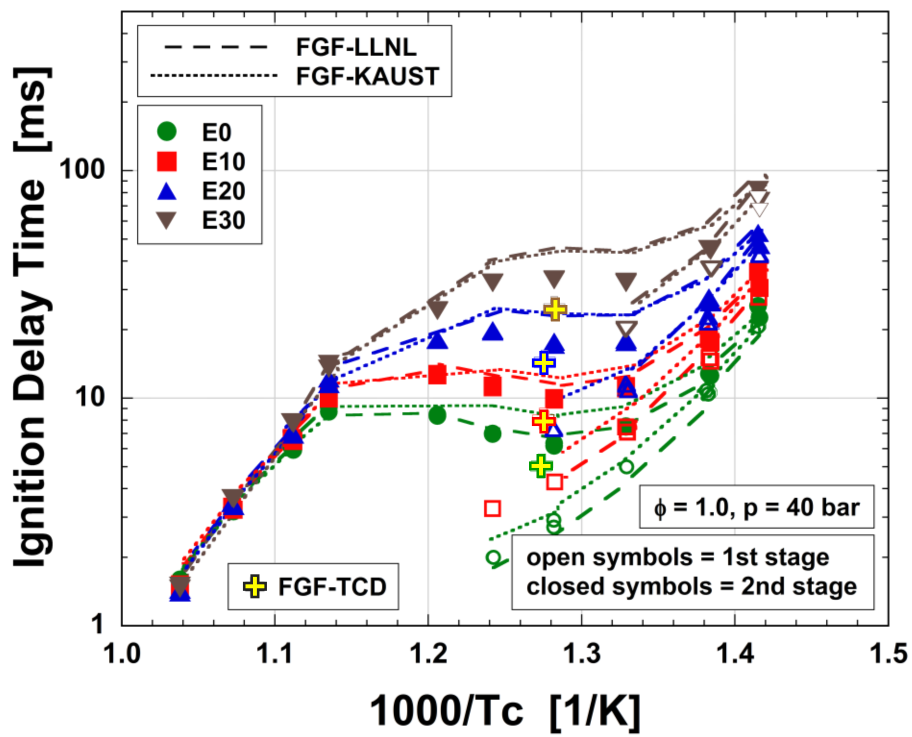
Functional Group	FACE-F	Target	FGF-TCD3
Paraffinic CH_3	41.03%	42.25	41.42
Paraffinic CH_2	19.44	19.4	19.94
Paraffinic CH	10.28	10.01	10.04
Paraffinic qC	5.48	5.08	4.75
Aromatic CH	5.26	5.24	5.55
CH_3 alpha to Aromatic	2.19	2.13	2.25
Aromatic qC	2.38	2.33	2.46
CH_2 alpha to Aromatic	0.19	0.20	0.21
Olefin CH	1.42	1.43	1.66
Olefin CH_2	1.43	1.43	1.66
Cyclic CH_2	10.90	10.52	10.04

TECHNICAL ACCOMPLISHMENTS / PROGRESS

Task 1 – Gasoline / Ethanol Blends

- Autoignition behavior experimentally <u>measured</u> for FACE-F, surrogates
  - Tc = 690–980 K, Pc = 21, 40 bar, ϕ = 1, E0–E30;
  - Influence of ethanol blending into surrogates is most significant at NTC, low-temperature conditions;
  - FGF-TCD3 appears somewhat more reactive than FACE-F, but trends with ethanol blending seem to be better captured.

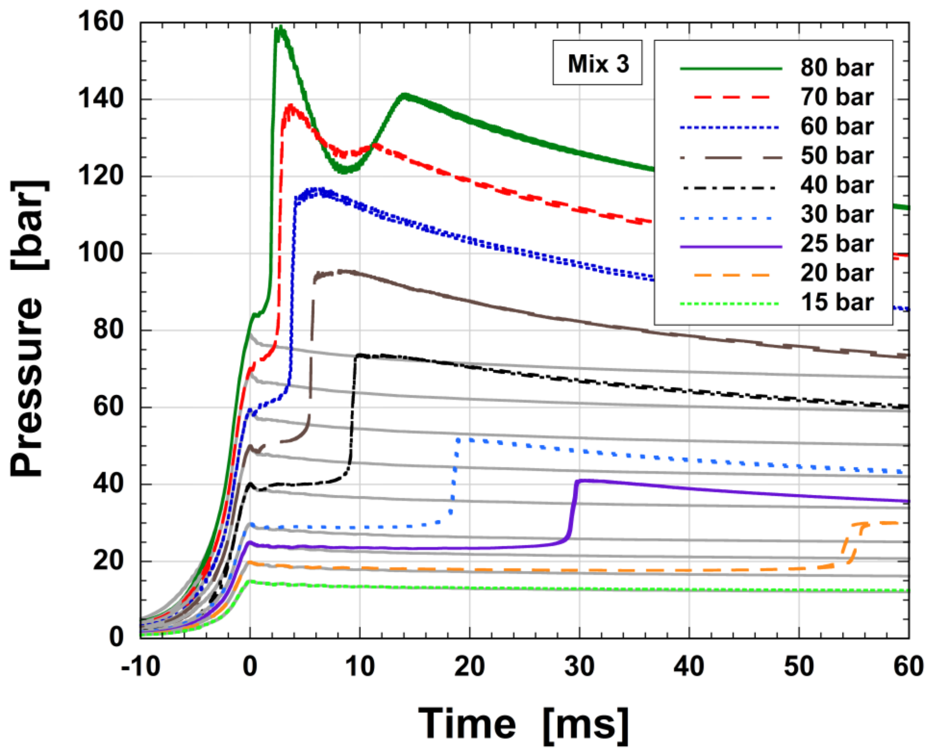


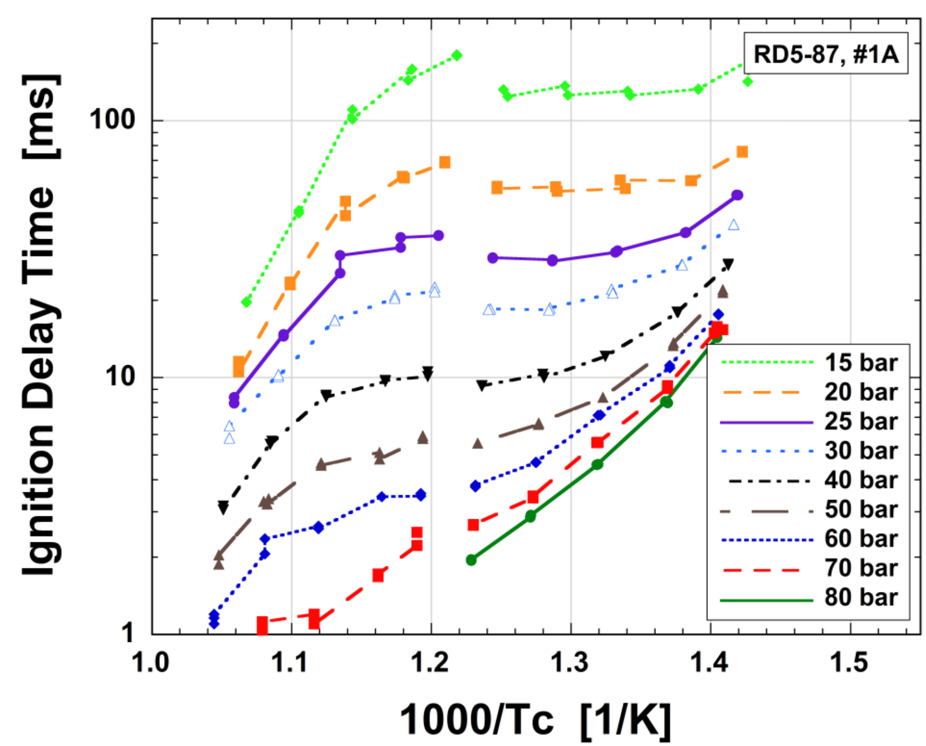


TECHNICAL ACCOMPLISHMENTS / PROGRESS

Task 2 – Measurements with RD5-87 (87 AKI / E10 gasoline)

- Tests conducted for surrogate development / kinetic model validation, and to gain insight into autoignition / performance in SNL LTGC engine
- Wide range of stoichiometries, compressed temperatures / pressures
- Analysis of measurements undertaken to quantify influences on ignition times, rates / extents of heat release

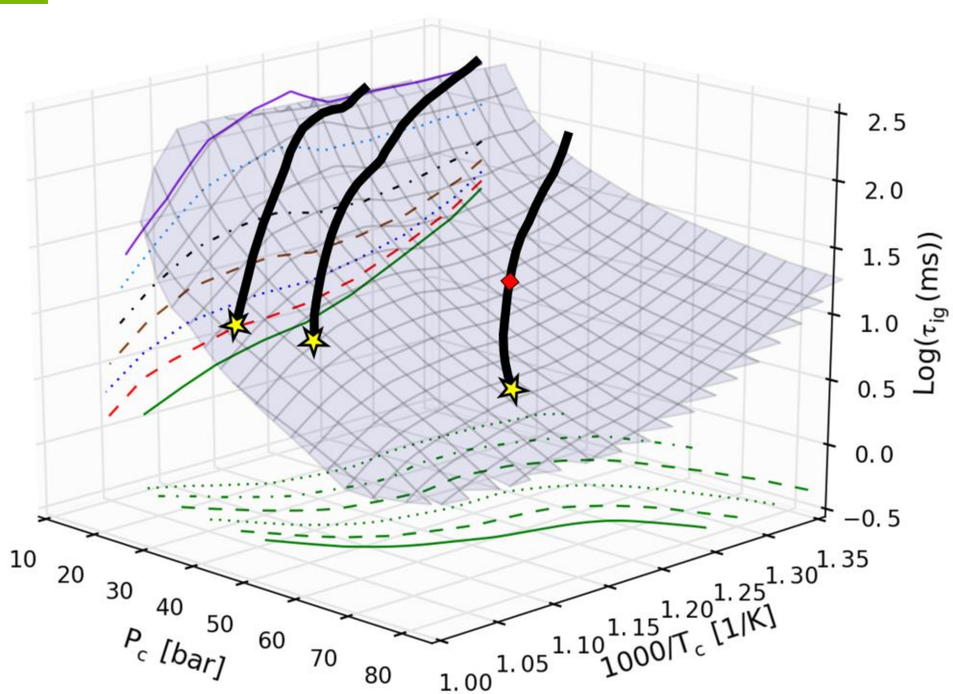


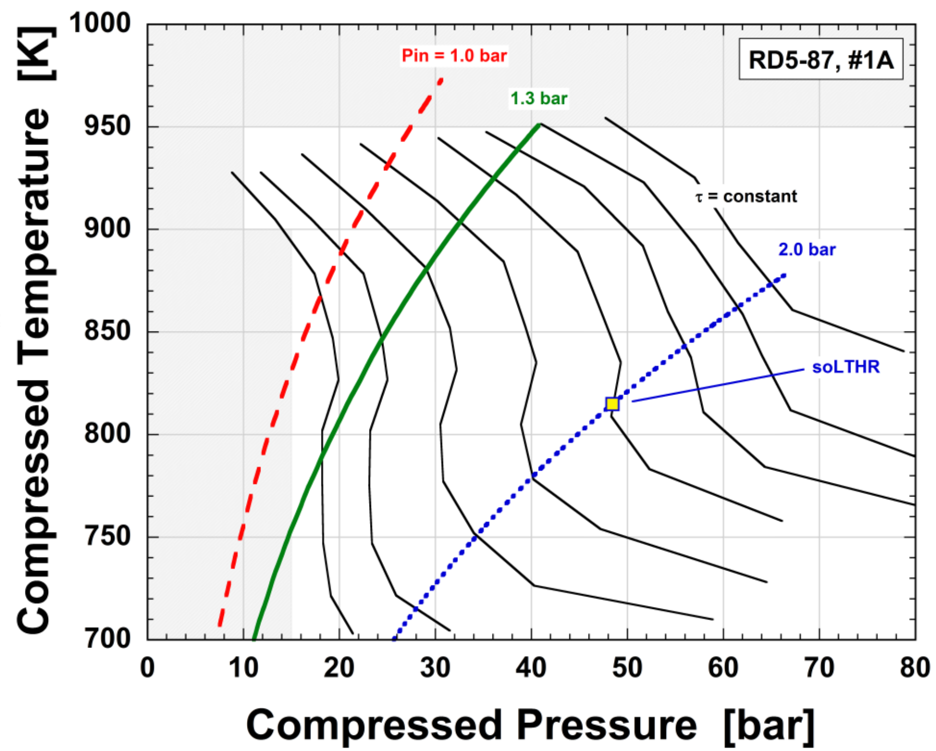


TECHNICAL ACCOMPLISHMENTS / PROGRESS

Task 2 – Measurements with RD5-87 (87 AKI / E10 gasoline)

- Autoignition behavior can be expressed as reactivity map where SNL LTGC in-cylinder conditions are projected to understand evolution of LTHR, shifts in CA10 as intake pressure is boosted
  - Transition from intermediate-temperature chemistry regime at Pin < 1.3 bar to NTC regime at Pin = 2.0 bar is identifiable in RCM results

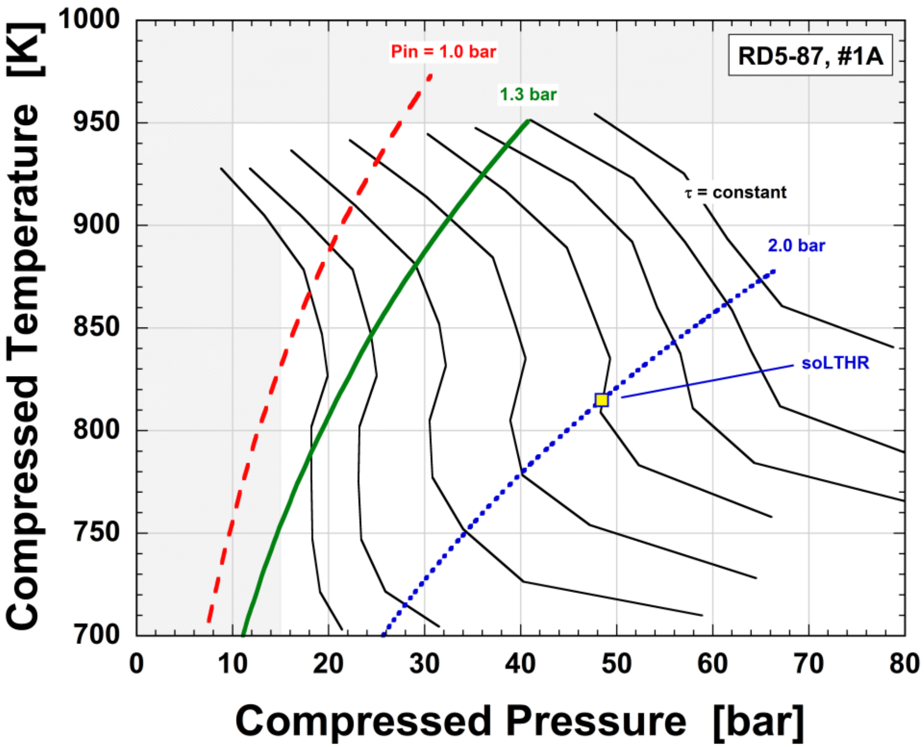


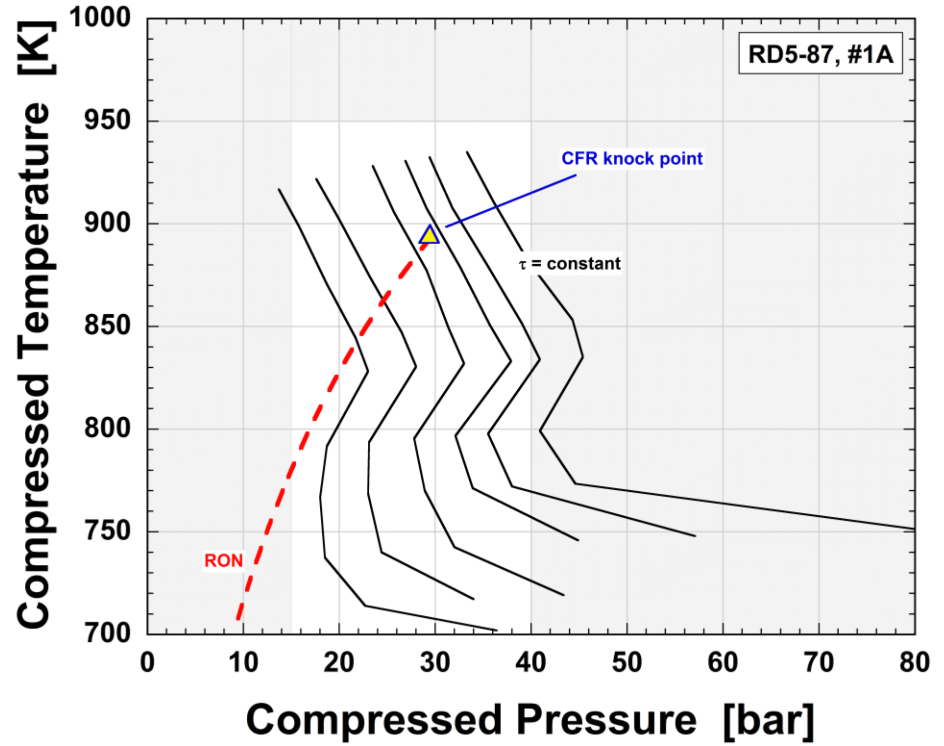


TECHNICAL ACCOMPLISHMENTS / PROGRESS

Task 2 – Measurements with RD5-87 (87 AKI / E10 gasoline)

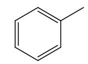
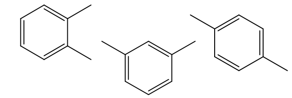
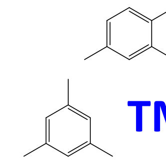
- RCM tests across other fuel-loading conditions can quantify shifts in reactivity (e.g., ignition timing (CA10, knock point), LTHR/ITHR)
  - projection to other engine operating schemes, e.g., RON test schedule, facilitates modeling, and understanding of dominant autoignition chemistries



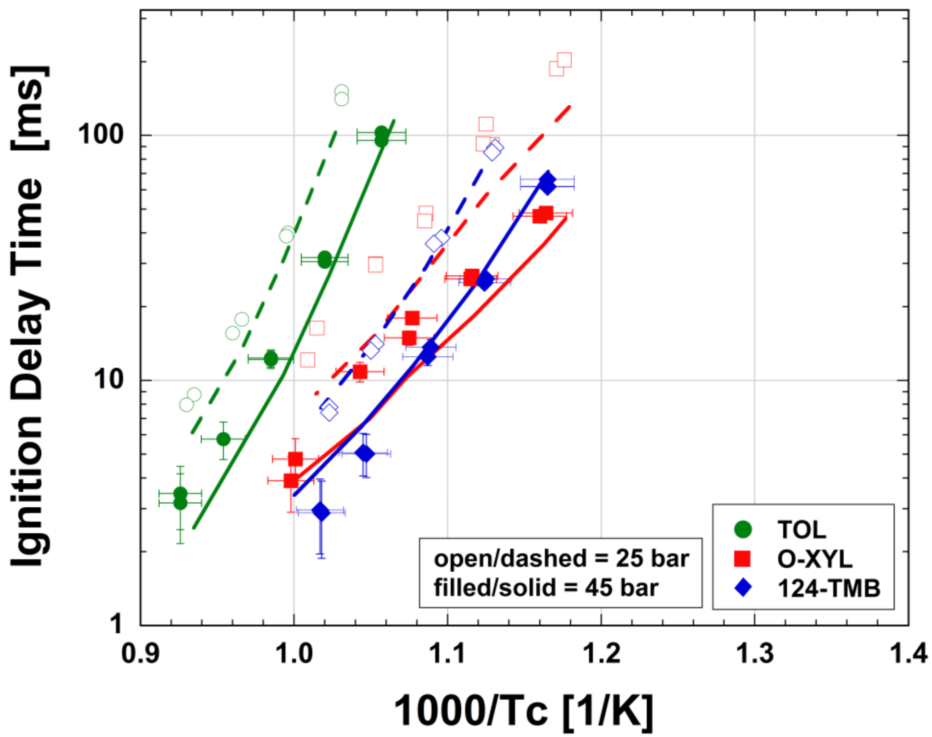


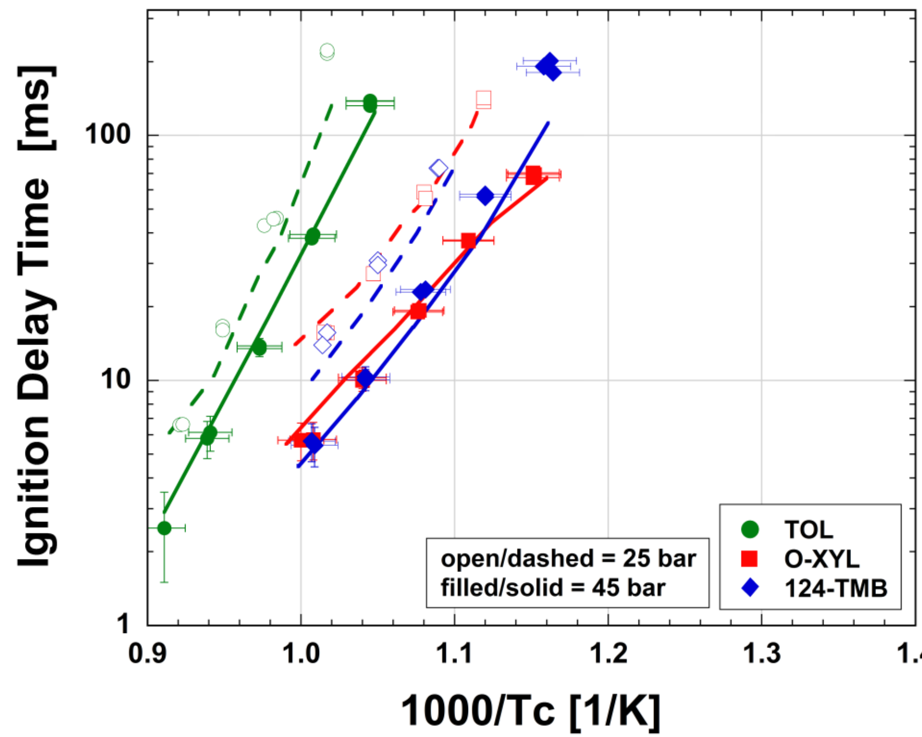
TECHNICAL ACCOMPLISHMENTS / PROGRESS

Task 4 – methylated aromatics


TOL

XYL

TMB

- Mono-aromatics are major constituents of real fuels
- Fundamental tests require lean/diluted mixtures at high pressure
  - Reactivity strongly dependent on temperature, weak sensitivities to ϕ
  - TOL is least reactive; O-XYL / 124-TMB are similarly reactive
- Comparisons with updated LLNL model demonstrates good agreement



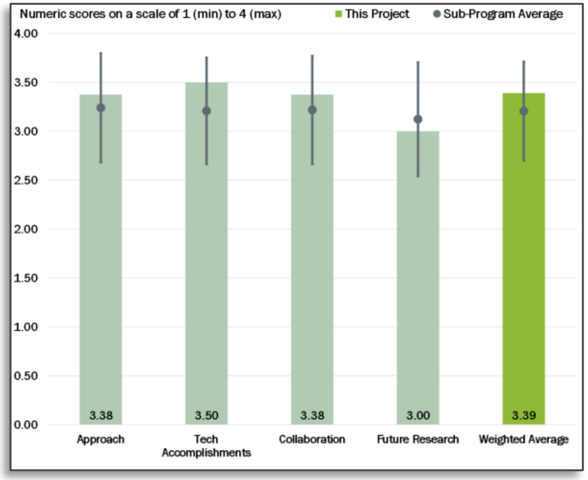


TECHNICAL ACCOMPLISHMENTS / PROGRESS

Task 5 – International RCM Workshop

- Data from many facilities used for kinetic model development
  - RCMs and shock tubes cover a wide range of engine-relevant conditions
- 2nd Characterization Initiative created to better understand and quantify facility influences, and platform-to-platform differences
  - To-date, contributions from 10 facilities worldwide using ethanol/'air', T_c = 780–1100 K, P_c = 20, 40 bar; non-reacting / reacting test measurements
  - Further confirm primary causes of machine-to-machine differences
  - Are there ways to modify design / operating protocol for more consistency?
  - Identify / promote 'Best Practices' for reporting / archiving datasets (collaborate with EU COST SmartCats Program WG4)
- Computational Fluid Dynamics Initiative
  - Enhance understandings of machine-to-machine, test-to-test differences
  - Explore challenges with advanced diagnostics implementation
    - Intrusive (e.g., physical sampling) and non-intrusive (laser-based)
  - Identify / promote 'Best Practices' for modeling of RCM experiments

RESPONSE TO REVIEWER COMMENTS



- This work positively impacts DOE objectives. It is extremely important for the development of chemical kinetic models at conditions representative of modern combustion strategies. Important data is provided for full boiling range fuels, surrogates and ethanol mixtures. It is important to support data that feeds kinetic modelers at LLNL, especially for problems that are most relevant to that team. The project is well-designed and well-integrated with other efforts (academia, national laboratories, and industry).
- The PI put tremendous effort to organize the RCM Workshop, which is critical to understanding of RCMs and providing high-fidelity RCM data. The work to consolidate data across multiple RCMs is welcome.
- The proposed future work could have been more descriptive, concerning fuels, blends and engine conditions. In addition, more detail concerning what else RCM data can do (beyond ignition delay and intermediate species measurement) to advance our knowledge of combustion in internal combustion engines and ultimately, advanced engine technology. The project team should interact with universities that have common interests outside of the RCM Workshop, especially considering budgetary constraints.
  - The project team at ANL actively coordinates with the LLNL groups focused on chemical kinetic modeling, and advanced numerical tools. This extensive collaboration is leveraged to ensure that RCM experimental campaigns target fuels and conditions needed to address model deficiencies (such as methylated aromatics in FY18), and thus model improvement. These interactions are ongoing, so flexibility is needed in test selection. New computational tools and algorithms are used to understand features such as heat release rates over a range of fuels and operating conditions.
  - The project team is demonstrating how reactivity maps derived from the measurements can be used to interpret engine behavior.
  - The PI collaborates with numerous universities, including sitting on PhD committees.

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COLLABORATIONS

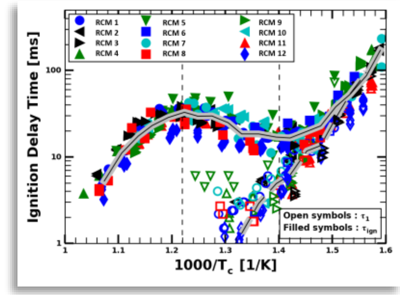
Ongoing Interactions (Inside / Outside VTO)

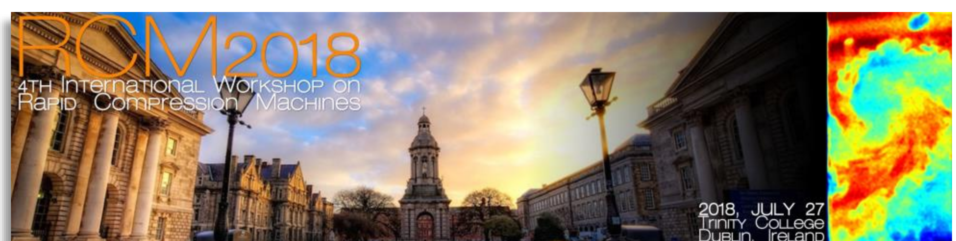
- DOE Working Groups: share data at meetings of AEC MOU, Co-Optima teams
- CRC FACE Working Group: participate in meetings; testing of AVFL-20 fuels
- ANL: gasoline LTC engine sharing data; refining UQ/GSA approaches to target reactions for mechanism improvement
- LLNL: kinetic model development / validation; formulation of gasoline surrogates; ToolKit development / testing
- SNL: LTGC engine data with RD5-87; tests with surrogate molecules
- Trinity College Dublin: functional-group basis for surrogate formulation
- RCM Workshop: facility-to-facility influences; 'Best Practices' (data reporting/archiving standards); advanced diagnostics implementation
- Other organizations: NUI Galway (kinetic models, similar fuel testing); Vrije Universiteit Brussel (CFD, reduced-order physical models); ETH-Zürich (DNS of RCM/autoignition processes); Danmarks Tekniske Universitet (PhD exchange student); Stanford/VUB/ETH-Zürich/U. Melborne (PhD examiner)

COLLABORATIONS

Community-wide Activities

- ANL-led, International RCM Workshop to better understand autoignition chemistry, turbulence-chemistry interactions, etc. using RCMs
  - Participation includes experimentalists, modelers, theoreticians
  - Establishing consensus for ‘Best Practices’
    - → Approaches for reporting / analyzing / comparing data
    - → Approaches for simulating the experiments
    - → Uncertainty quantification for experiments and modeling
    - → Regimes of overlap with other experimental devices
  - CFD (MZM, RANS, LES, DNS) to explore measurement challenges
  - 4th Workshop to be held 27 July 2018 at Trinity College Dublin, IRELAND (in conjunction with Int. Combustion Symposium, TNF, ISF, Flame Chemistry…)





REMAINING CHALLENGES / BARRIERS

- Understanding and representing the autoignition characteristics of full boiling range fuels, blending with ethanol, etc., via multiple-component (3-10) surrogate mixtures requires improved capabilities to formulate surrogates, considering new methods and surrogate components;
- Improvements to gasoline surrogate model require deeper understanding of mechanism behavior, and uncertainties associated with low temperature chemistry pathways of base model;
- Ignition delay time and preliminary heat release are integrated metrics for ignition chemistry, constraints exist with their utility; additional diagnostics, like heat release rates, measurement of chemical intermediates, etc., could improve development / validation efforts.

PROPOSED FUTURE WORK

FY 2018 and beyond

- Proposed future work is subject to change based on funding levels
- Physical testing of multi-component surrogates (FACE-F, etc.), leveraging interactions with LLNL / others, to improve robustness of formulations
  - Utilize novel techniques / targets to select component molecules, blending ratios, including blends with ethanol;
  - Understand chemical kinetic interactions between neat fuel and ethanol.
- Conduct RCM tests to quantify effects of exhaust gas recirculation (EGR)
  - Coordinate with SNL to target LTGC engine conditions (T, P, ϕ, EGR) using RD5-87 (E10 certification gasoline);
  - Coordinate with LLNL to formulate and test surrogate blends for RD5-87.
- Additional measurements of aromatic surrogates, binary blends with olefins to probe synergistic/antagonistic behavior
  - Coordinate with LLNL for model development
- Extend UQ/GSA to additional targets such as heat release rates, reaction intermediates

PROPOSED FUTURE WORK

FY 2017 and beyond

- Conduct further tests with CRC AVFL-20 fuels
  - Coordinate with MIT, AVFL-30 committee to better understand / interpret measurements across RCM and spark-ignition engine platforms considering knock-limited performance
- Continue co-ordination of International RCM Workshop

SUMMARY

- Objective
  - Acquire data, validate / improve models for transportation-relevant fuels
- Project Approach
  - Utilize ANL's RCM and novel analysis tools, leverage expertise of DOE-funded researchers to synergistically improve predictive models
- Technical Accomplishments / Progress
  - Acquired data to understand autoignition behavior of multi-component surrogate blends for gasolines, including ethanol blends (E0–E30);
  - Identified fuel, mixture and operational parameters controlling mild ignition;
  - Hierarchically identified facility influences on RCM measurements.
- Collaborations
  - National labs, universities and industry; International RCM Workshop
- Future Work
  - Testing with gasoline surrogate components, blends and full boiling range gasolines across engine-relevant (T, P, ϕ, EGR) conditions;
  - Advances / improvement in UQ/GSA, covering additional targets.

THANK YOU

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